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Perturbation method for non-square Hamiltonians and its application to polynomial oscillators

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Abstract

A remarkable extension of Rayleigh-Schrödinger perturbation method is found and described. Its $(N+q)\times(N+1)-$dimensional Hamiltonians are assumed emerging during quasi-exact constructions of bound states. At all $q>1$, the role of the traditional single eigenvalue is taken over by an energy/coupling $q-$plet. In a way circumventing both the non-linearity and non-Hermiticity difficulties, the corrections are defined by compact, $q-$dimensional matrix-inversion formulae.

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1 Introduction

The existence and efficiency of several sufficiently simple perturbation techniques represents one of the not entirely negligible reasons why the abstract formalism of Quantum Theory finds so numerous and impressive practical applications. Usually, one is given a "realistic" (i.e., quite often, fairly complicated) Schrödinger equation

$$(H-E)\,|\psi\rangle = 0$$

and succeeds in its approximative replacement by a significantly simpler equation

$$\left(H^{(0)}-E^{(0)}\right)\,|\psi^{(0)}\rangle = 0$$

where

(1) the difference between the "correct" and "approximate" measurable quantities (here, between energies E_n and $E_n^{(0)}$ at a few level-indices n) proves small,

(2) the latter, "zero-order" problem is comparatively easy to solve, and

(3) a suitable (e.g., Rayleigh-Schrödinger [1]) version of the so called perturbation theory is found as a source of a recipe for a systematic improvement of the approximation.

In a broader perspective, one may keep the energy E fixed and switch to a modified Schrödinger operator, $H-E=H'(E)-gV=H''-S(E,g)=\ldots$. An appropriately modified perturbation theory might then serve as a tool for the determination of the "fine-tuned" couplings g [2] or, whenever necessary, of the whole multiplets of the couplings $g_1,\ g_2,\ldots,g_{q-1}$ which may even re-incorporate the energy itself by putting, formally, $E\equiv -g_0$. In the latter setting the "original" or "realistic" problem quite often acquires the "$q-$plet-eigenvalue" generalized form

$$[H-S(g_0,g_1,\ldots,g_{q-1})]\,|g_0,g_1,\ldots,g_{q-1}\rangle = 0 \tag{1}$$

which will be considered and studied in what follows.

2 Polynomial-oscillator sample of equation (1)

Differential Schrödinger equation

$$-\psi''(x)+V(x)\,\psi(x)=E\,\psi(x) \tag{2}$$

for a particle moving in a one-dimensional polynomial well

$$V(x) = g_1 x^2 + g_2 x^4 + \ldots + g_{2q+1} x^{4q+2}, \qquad g_{2q+1} > 0 \tag{3}$$

may be used as an illustrative example. Its solutions prove often tractable via the infinite Taylor series

$$\psi(x) = \exp[-P(x)] \times \sum_{n=0}^{\infty} h_n x^{2n+p} \tag{4}$$

where the integer $p = 0$ or 1 characterizes the parity. It may be re-interpreted as an angular momentum $\ell = p - 1 = 0, 1, \ldots$ in three dimensions, etc.

In place of the general exponent $P(x)$ we shall only use here a polynomial

$$P(x) = \sum_{k=0}^{q} \frac{x^{2k+2}}{2k+2} \, f_k \, . \tag{5}$$

The asymptotically optimal choice of its coefficients f_k is uniquely determined by the WKB condition

$$V(x) = [P'(x)]^2 + \mathcal{O}\left(x^{2q}\right) \tag{6}$$

or, if you wish,

$$g_{2q+1} = f_q^2, \quad g_{2q} = 2 f_q f_{q-1}, \; \ldots, \quad g_{q+1} = \sum_{j=0}^{q} f_{q-j} f_j \tag{7}$$

which fixes all the $q+1$ coefficients f_k as functions of the first $q+1$ dominant couplings g_{2q+1}, g_{2q}, $\ldots$, g_{q+1} in potential (3). Thus, we have $f_0 = \sqrt{g_1}$ for harmonic oscillator ($q = 0$) or $f_1 = \sqrt{g_3}$ and $f_0 = g_2/(2f_1)$ for the sextic anharmonic oscillator ($q = 1$) etc.

The insertion of (4) transforms our differential Schrödinger eq. (2) + (3) into the infinite-dimensional matrix problem (1) where the non-square matrix of the system possesses the $(q+2)-$diagonal banded form,

$$H - S(g_0, g_1, \ldots, g_{q-1}) = \begin{pmatrix} B_0 & C_0 & & & & & & \\ A_1^{(1)} & B_1 & C_1 & & & & & \\ \vdots & \ddots & \ddots & \ddots & & & & \\ A_q^{(q)} & \cdots & A_q^{(1)} & B_q & C_q & & & \\ & \ddots & & \ddots & \ddots & \ddots & & \\ & & A_m^{(q)} & \cdots & A_m^{(1)} & B_m & C_m & \\ & & & \ddots & & \ddots & \ddots & \ddots \end{pmatrix} . \tag{8}$$

The g_k-dependence of the matrix elements is transparent,

$$
\begin{aligned}
C_n = (2n+2)\,(2n+2p+1), \qquad & B_n = -g_0 - f_0\,(4n+2p+1) \equiv A_n^{(0)},\\
A_n^{(1)} = -f_1\,(4n+2p-1) + f_0^2 - g_1, \qquad & A_n^{(2)} = -f_2\,(4n+2p-3) + 2f_0f_1 - g_2,\\
& \ldots,\\
A_n^{(q)} = -f_q\,(4n+2p+1-2q) + (f_0f_{q-1} + f_1f_{q-2} + \ldots + f_{q-1}f_0) - g_q, & \\
n = 0, 1, \ldots &
\end{aligned}
\tag{9}
$$

(remember that $-g_0 \equiv E$ is the energy). We have

$$
S(g_0, g_1, \ldots, g_{q-1}) = \sum_{\xi=1}^{q} g_{\xi-1}\mathcal{J}_\xi \tag{10}
$$

where the generalized vectorial eigenvalue $\vec{g} = \{g_0, g_1, \ldots, g_{q-1}\}$ is attached to a $q-$plet of auxiliary one-diagonal unit-like infinite-dimensional matrices $\mathcal{J}_\xi$.

2.1 Illustration: $q = 0$ (harmonic oscillator)

At $q = 0$ we may re-scale the coordinate x and set $V(x) = x^2$ and $g_1 = f_0 = 1$ giving $\psi(x) = \exp(-x^2/2) \times \ldots$ etc. From the formal secular equation

$$
\det\left[H - S(g_0)\right] = \det \begin{pmatrix} B_0 & C_0 & & \\ 0 & B_1 & C_1 & \\ & \ddots & \ddots & \ddots \end{pmatrix} = 0, \qquad q = 0
$$

we deduce that the harmonic-oscillator spectrum is reproduced once we let the secular determinant vanish by setting one of its diagonal elements B_m equal to zero. Thus, the $q = 0$ example may be skipped as trivial in what follows.

3 Magyari's finite-dimensional equations (1)

In a pioneering letter [3], E. Magyari discovered the existence of the so called quasi-exact [4] bound states in some special cases of the general polynomial potential wells (3). In our present language, his claim is that the infinite-dimensional matrix-equation representation (1) + (8) of the polynomial oscillators admits a rigorous

and exact finite-dimensional truncation. We only have to select the very specific truncation-compatible "intermediate" coupling

$$g_q = -f_q\,(4N+2q+2p+1) + (f_0 f_{q-1} + f_1 f_{q-2} + \ldots + f_{q-1} f_0) \tag{11}$$

in order to arrive at the finite-dimensional matrices in eq. (1),

$$H-S = \left(\begin{array}{ccccccccc}
B_0 & C_0 & & & & & & & \\
A_1^{(1)} & B_1 & C_1 & & & & & & \\
\vdots & \ddots & \ddots & \ddots & & & & & \\
A_q^{(q)} & \cdots & A_q^{(1)} & B_q & C_q & & & & \\
 & \ddots & & \ddots & \ddots & \ddots & & & \\
 & & A_{N-2}^{(q)} & \cdots & A_{N-2}^{(1)} & B_{N-2} & C_{N-2} & & \\
 & & & A_{N-1}^{(q)} & \cdots & \ddots & B_{N-1} & C_{N-1} & \\
 & & & & \ddots & \ddots & \vdots & B_N & \\
 & & & & & A_{N+q-2}^{(q)} & A_{N+q-2}^{(q-1)} & \vdots & \\
 & & & & & & A_{N+q-1}^{(q)} & A_{N+q-1}^{(q-1)} &
\end{array} \right). \tag{12}$$

At every choice of the integer $N = 0, 1, 2, \ldots$ it makes sense to contemplate the next, $\mathcal{O}\,(x^{2q})$ order of precision in our WKB formula (6). This leads to eq. (11) and connects the value of the subdominant coupling g_q with the $x^{2N+p}-$dominated truncated wave functions (4).

We get $A_n^{(q)} = 4\,f_q\,(N+q-n)$ and reduce the original infinite-dimensional linear algebraic system (1) to its finite-dimensional subset which consists of the mere $N+q$ rows. As long as we assumed that $h_{N+1} = h_{N+2} = \ldots = 0$, only the $N+1$ Taylor coefficients $h_0, h_1, \ldots, h_N$ remain unknown and must be determined by eq. (1). In this sense the latter equation is overcomplete and, in effect, non-linear. The operator $H-S$ becomes represented by a non-square, $(N+q)\times(N+1)-$dimensional matrix.

3.1 Sextic quasi-exact oscillators ($q=1$ and all $N=0,1,\ldots$)

At the first nontrivial $q=1$ we may re-scale the coordinate x and pick up, say, the even parity $p=0$. This gives $V(x) = x^6 + 2f_0x^4 + (f_0^2 - 3 - 4N)x^2$ and the bound states $\psi(x) = \exp(-x^4/4 - f_0x^2/2) \times \ldots$. One arrives at the *square-matrix* secular

equation of the $N+1-$dimensional form

$$\det\left[H-S(g_0)\right]=\det\left(\begin{array}{ccccc} B_0 & C_0 & & & \\ A_1^{(1)} & B_1 & C_1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & B_{N-1} & C_{N-1} \\ & & & A_N^{(1)} & B_N \end{array}\right)=0, \qquad q=1\,.$$

The standard square-matrix techniques may be employed so that also all the quasi-exact constructions of the sextic oscillators with $q=1$ may be skipped here as a mere routine exercise.

3.2 Explicit solution at $N=0$ and all q

Once we contemplate the higher degrees $q=2,3,\ldots$ in our quasi-exact polynomial-oscillator Schrödinger-Magyari non-square-matrix bound-state problem (1) + (12), we must admit that their solution represents a challenge. The only manifestly non-numerical example occurs at $N=0$ where the solution remains elementary,

$$E=-g_0=f_0\,(2p+1), \qquad g_1=f_0^2-f_1\,(2p+3), \qquad \ldots,$$
$$g_{q-1}=(f_0f_{q-2}+f_1f_{q-3}+\ldots+f_{q-2}f_0)-f_{q-1}\,(2p+2q-3), \qquad N=0.$$

The asymptotically dominant couplings $g_{2q+1},g_{2q},\ldots,g_{q+1}$ in the potential (3) remain freely variable while the $q+1$ elements of the remaining set $g_0,g_1,\ldots,g_q$ become fixed as their explicit quadratic functions. One may preserve such a pattern in all the $N\geq 1$ cases.

3.3 A toy decadic example: $q=2$ and $N=2$.

Before we get to the core of our present message and formulate the general perturbation method of solving eq. (1) at the arbitrarily large integers $q\geq 2$ and $N\geq 1$, let us emphasize that the *idea* of the method may be most easily illustrated by its application to the elementary decadic models with $q=2$ and with the re-scaled x such that $f_2=\sqrt{g_5}=1$. The two free parameters f_1 ($\equiv g_4/2$) and f_0 [$\equiv (g_3-f_1^2)/2$] define $g_2=2f_0f_1-2p-13$ [cf. eq. (11)] and exponent $P(x)$ [cf. eq. (5)]. They also

occur in the matrix elements of eq. (1) which reads

$$\left(\begin{array}{ccc} -g_0-f_0-2pf_0 & 2+4p & 0 \\ f_0^2-g_1-3f_1-2pf_1 & -g_0-5f_0-2pf_0 & 12+8p \\ 8 & f_0^2-g_1-7f_1-2pf_1 & -g_0-9f_0-2pf_0 \\ 0 & 4 & f_0^2-g_1-11f_1-2pf_1 \end{array}\right)\left(\begin{array}{c} h_0 \\ h_1 \\ h_2 \end{array}\right)=0 \tag{13}$$

and which should determine the two unknown eigenvalues g_0 (representing the negative energy) and g_1 (= the non-variable coupling at x^2) as well as the two coefficients h_0 and h_1 in the wave function (note that $h_2 = 1$ is a mere fixed normalization constant).

4 Perturbation forms of Magyari's equations (1)

Studies of analytic potentials found a mathematical encouragement in the Regge's complex angular momentum method [5]. In this context, our parity parameter could be prolonged to the *complex* angular momentum $\ell \equiv p-1 \in \mathbb{C}$. Rather unexpectedly, the resulting extension of the range of p will enable us to simplify the bound-state problem (1) + (12) in the limit of the large $|p| \gg 1$ [6]. Let us now outline the two alternative possibilities of such a simplification in some detail.

4.1 An elementary large$-\ell$ model

In the toy example of paragraph 3.3 let us introduce the quantity $\lambda = 1/(2p)$ and assume that the numerical value of this λ may be chosen arbitrarily small. This implies that the identical decomposition

$$H = 2p\left[H^{(0)} + \lambda\, H^{(1)}\right], \qquad q = N = 2 \tag{14}$$

of our Hamiltonian in eq. (13) with

$$H^{(0)} = \left(\begin{array}{ccc} -f_0 & 2 & 0 \\ -f_1 & -f_0 & 4 \\ 0 & -f_1 & -f_0 \\ 0 & 0 & -f_1 \end{array}\right) \quad \text{and} \quad H^{(1)} = \left(\begin{array}{ccc} -f_0 & 2 & 0 \\ f_0^2-3f_1 & -5f_0 & 12 \\ 8 & f_0^2-7f_1 & -9f_0 \\ 0 & 4 & f_0^2-11f_1 \end{array}\right)$$

acquires the manifestly perturbative character. The dominant $H^{(0)}$ is a very simple tridiagonal matrix while the more complicated and four-diagonal matrix $H^{(1)}$ remains

tractable as a mere perturbation. Thus, the current conditions of the applicability of perturbation algorithms are satisfied. We may expect that at the larger integers q and/or N, the same pattern will enable us to postulate the formal split of any given non-square Hamiltonian H in some formal Taylor series

$$H = H^{(0)} + \lambda\, H^{(1)} + \lambda^2\, H^{(2)} + \ldots \tag{15}$$

where the choice of the "sufficiently small" parameter λ is arbitrary. Even in the present letter this quantity may be re-defined as $\lambda = 1/(2p + const)$, in the spirit of the popular "shifted large$-\ell$" expansions [7].

4.2 A more advanced large$-\ell$ arrangement of the same model

Let us abbreviate $-g_0 - 2pf_0 = 2pE$, $f_0^2 - g_1 - 2pf_1 = 2pF$ and re-scale eq.(13),

$$\left[\mathcal{T}\left(\begin{array}{ccc} 2pE - f_0 & 2+4p & 0 \\ 2pF - 3f_1 & 2pE - 5f_0 & 12+8p \\ 8 & 2pF - 7f_1 & 2pE - 9f_0 \\ 0 & 4 & 2pF - 11f_1 \end{array}\right)\mathcal{S}\right]\left[\mathcal{S}^{-1}\left(\begin{array}{c} h_0 \\ h_1 \\ h_2 \end{array}\right)\right] = 0 \tag{16}$$

with the "small" $\sigma = p^{-1/3}$ in

$$\mathcal{T} = \left(\begin{array}{cccc} \sigma^{-1}/(4p) & & & \\ & \sigma^{-2}/(4p) & & \\ & & \sigma^{-3}/(4p) & \\ & & & \sigma^{-4}/(4p) \end{array}\right) \quad \text{and} \quad \mathcal{S} = \left(\begin{array}{ccc} 1 & & \\ & \sigma & \\ & & \sigma^2 \end{array}\right).$$

This leads to another re-formulation of our problem (16),

$$[H - S(s,t)]\;|s,t\rangle = 0, \qquad |s,t\rangle = \mathcal{S}^{-1}\left(\begin{array}{c} h_0 \\ h_1 \\ h_2 \end{array}\right), \qquad s = -\frac{E}{2\sigma}, \qquad t = -\frac{F}{2\sigma^2} \tag{17}$$

and to another perturbation arrangement (15) of the Hamiltonian where the new unperturbed Hamiltonian

$$H^{(0)} = \left(\begin{array}{ccc} 0 & 1 & 0 \\ 0 & 0 & 2 \\ 2 & 0 & 0 \\ 0 & 1 & 0 \end{array}\right) \tag{18}$$

is accompanied by the three non-vanishing one-diagonal matrix correction coefficients in eq. (15) with $\lambda \equiv \sigma = p^{-1/4} \ll 1$,

$$H^{(1)} = -\frac{f_1}{4}\begin{pmatrix} 0 & 0 & 0 \\ 3 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 11 \end{pmatrix}, \quad H^{(2)} = -\frac{f_0}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 9 \\ 0 & 0 & 0 \end{pmatrix}, \quad H^{(3)} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 6 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The eigenvector $|s,t\rangle$ as well as the eigenvalue matrix S in eq. (17) should be also represented by the infinite Taylor-series ansatzs

$$S = S^{(0)} + \lambda\, S^{(1)} + \lambda^2\, S^{(2)} + \dots \tag{19}$$

and

$$|s,t\rangle = |s^{(0)},t^{(0)}\rangle + \lambda\, |s^{(1)},t^{(1)}\rangle + \dots\,. \tag{20}$$

The key specific merit of such a sophisticated innovation lies in an unexpected and very significant simplification of the zero-order (i.e., $|p| \to \infty$ limit of) Schrödinger-Magyari equations. For more details we may either refer to our older paper [8] or to the Appendix A where a few more technical details are summarized. These details are instructive since our particular $q = N = 2$ zero-order concrete model (18) admits a straightforward generalization to all N, at $q \leq 5$ at least [6].

5 The evaluation of perturbation corrections

The generic infinite-dimensional matrix equation (1) may be solved, say, by the technique of the so called vectorial continued fractions [9]. Perturbation re-arrangements of such a treatment of our problem exist but still carry a more or less purely numerical character [10]. Here, an entirely different approach is being employed.

For the sake of definiteness, we shall only pay attention to the Magyari's finite-dimensional constructions at arbitrary truncation integers $N < \infty$. The scope of the method might be broader in principle but we decided to consider the Magyari's problem only. Indeed, due to the practical difficulties with its solution it hardly possesses any applications beyond the first few qs *or* Ns at present.

As we already indicated, our present approach to the Magyari's problem (1) (we may call it "perturbed" problem) will be perturbative. We shall postulate

$$|g_0, g_1, \dots, g_{q-1}\rangle = |g_0^{(0)}, g_1^{(0)}, \dots, g_{q-1}^{(0)}\rangle + \lambda\, |g_0^{(1)}, g_1^{(1)}, \dots, g_{q-1}^{(1)}\rangle + \dots \tag{21}$$

and employ the parallel expansion (20) of the $q-$plet of eigenvalues which contains $S = S(g_0, g_1, \ldots, g_{q-1})$ and $S^{(k)} = S({g_0}^{(k)}, {g_1}^{(k)}, \ldots, g_{q-1}^{(k)})$ with $k = 0, 1, \ldots$.

We may re-write our "perturbed" Schrödinger equation (1) order-by-order in λ. One expects that for the study of similar equations, all the solutions are at our disposal not only for the overcomplete zero-order equation

$$H^{(0)}\,|g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}\rangle = S({g_0}^{(0)}, {g_1}^{(0)}, \ldots, g_{q-1}^{(0)})\,|g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}\rangle \qquad (22)$$

but also for its under-complete "left-action" partner

$$\langle_\xi\langle g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}|\,H^{(0)} = \langle_\xi\langle g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}|\,S({g_0}^{(0)}, {g_1}^{(0)}, \ldots, g_{q-1}^{(0)})\,. \qquad (23)$$

On the level of the first-order corrections we complement the zero-order homogeneous equation (22) by the *non-homogeneous* linear algebraic problem using an abbreviation $|\,0\rangle = |g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}\rangle$,

$$\left[H^{(0)} - S^{(0)}\right]|g_0^{(1)}, g_1^{(1)}, \ldots, g_{q-1}^{(1)}\rangle = \left[S^{(1)} - H^{(1)}\right]\,|\,0\rangle\,. \qquad (24)$$

Similarly we add its second-order descendant

$$\left[H^{(0)} - S^{(0)}\right]|g_0^{(2)}, g_1^{(2)}, \ldots, g_{q-1}^{(2)}\rangle = \left[S^{(1)} - H^{(1)}\right]\,|\,1\rangle + \left[S^{(2)} - H^{(2)}\right]\,|\,0\rangle \qquad (25)$$

(with abbreviated $|\,1\rangle = |g_0^{(1)}, g_1^{(1)}, \ldots, g_{q-1}^{(1)}\rangle$) and so on. All the equations in this hierarchy have the same recurrent structure,

$$\left[H^{(0)} - S^{(0)}\right]|\,k\rangle = |\,\mathrm{known}^{(k-1)}\rangle + S^{(k)}\,|\,0\rangle \qquad (26)$$

with "input" $|\,\mathrm{known}^{(0)}\rangle = -H^{(1)}\,|\,0\rangle$ at $k = 1$, etc.

This completes our description of the overall strategy and algorithm. In dependence on the particular features of $H^{(0)}$ and of its eigenstates, a few more detailed technical aspects of our innovated recipe may be added in a more explicit form which is $H^{(0)}-$dependent of course.

For our concrete construction of section 4.2 (which admits various generalizations [6]), the technical details are particularly rich and relevant and they contribute to a perceivable enhancement of the efficiency of the practical calculations. All of them may be found summarized in Apendix B which offers a slightly more formal reading.

6 Discussion and summary

6.1 The next-to-elementary quasi-exact bound states

In various applications of Quantum Mechanics people sometimes forget that the occurrence of the compact and elementary "user friendly" wave functions is not restricted to the mere linear harmonic oscillator $V(x) = x^2$. Due to Magyari [3] we know that the similar exceptional bound states, say, of the form

$$\psi_{(QE)}(x) = x^{\text{const}} \exp(-\text{polynomial}(x)) \times \text{polynomial}(x) \tag{27}$$

are much more generic and may be generated by virtually any polynomial potential at certain particular subsets of couplings and energies.

Unfortunately, all his formally flawless generalizations of the $q = 0$ harmonic oscillator to $q = 1, 2, \ldots$ found applications solely at $q = 1$ (cf., e.g., [11]). Certain $q = 2$ models attracted attention just at the very small N [12]. In all the other cases, the unfortunate coincidence of the nonlinearity and non-Hermiticity of H proved deterring. In this sense, our present new approach might re-vitalize interest in the undeniable phenomenological merits of the quasi-exact models with the larger qs and Ns.

In this direction we already re-analyzed a few particular non-square Magyari's equations (1) at the freely variable dimensions N and discovered, purely empirically, that some of these equations exhibit certain unexpected "user-friendly" features up to $q = 5$ at least [6]. Moreover, it has been established by several groups of authors that in a way paralleling the exceptional $q = 1$ oscillators, some of their "first nontrivial" $q = 2$ descendants *also* admit the existence of quasi-exact multiplets which may be arbitrarily large [13]. Efficiently, their non-Hermiticity may be tamed by an appropriate modification of the "physical" inner product in Hilbert space [14].

All these observations might revitalize interest of people in the Magyari's non-square matrix problem (1). In our present paper we demonstrated that in spite of its non-linearity, rather surprisingly, this anomalous form of the Schrödinger equation still admits a systematic perturbative solution. We believe that the resulting facilitated perturbative tractability might make Magyari's oscillators significantly more attractive in applications.

6.2 Innovations in perturbation theory

Perturbation analysis of nonlinear systems usually requires a narrow specification of their nonlinearity (cf., e.g., [15] for illustration). Hence, it was a nice feeling to reveal that the nonlinearity which characterizes the Magyari's equations (1) still does not prevent us from employing the ideas of the Rayleigh-Schrödinger perturbation construction of their solutions.

We should remind the readers that the use of the perturbation series is one of the most natural strategies, able to provide closed formulae as well as the upper and/or lower bounds of the measurable quantities [16]. Equally well it seems suitable for the study of the real and complex eigenvalues [17]. This puts our present perturbative approach to Magyari's problem into a broader context and comparison.

First of all, the specific merit and recommendation of our present approach for future calculations may be seen in the rapid growth of the complexity of the various non-perturbative alternative methods with the growth of N. Indeed, just the first few smallest integers N seem to have been considered in the "minimally nontrivial" $q = 2$ context up to now [18].

Secondly, our present method looks comparatively friendly also with respect to the growth of the integer q which measures the flexibility of the shape of the potential (3). In a way complementing and extending our thorough perturbation study at $q = 1$ [19], we showed here that an apparent incompatibility of the perturbation-expansion strategy with the Magyari's equations at the larger q proves false. We imagined that even some quite strongly non-square matrix forms of the Magyari's Hamiltonian matrices with $q > 2$ remain tractable when *both* their left and right action are taken into account *simultaneously*.

In this sense, a certain methodical gap has been filled by our present paper. Still, several open questions survive. For example, the finite-dimensional character of our present Hamiltonian matrices H might help to suppress the weight of some problems with convergence which often mar the use of the perturbation techniques for many infinite-dimensional Hs [20]. In particular, one might recollect the encouraging rigorous "acceleration of convergence" results as obtained at the "trivial" $q = 1$ in ref. [19].

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Appendix A: Zero-order example (18)

For the time being let us ignore the notation subtleties and changes of notation of section 4.2 and assume simply that a given toy unperturbed non-square Hamiltonian (18) may be assigned the generalized eigenvalues

$$S^{(0)}(g_0^{(0)},g_1^{(0)}) = \begin{pmatrix} {g_0}^{(0)} & & \\ {g_1}^{(0)} & {g_0}^{(0)} & \\ & {g_1}^{(0)} & {g_0}^{(0)} \\ & & {g_1}^{(0)} \end{pmatrix} \equiv {g_0}^{(0)}\mathcal{J}_1 + {g_1}^{(0)}\mathcal{J}_2$$

and eigenvectors

$$|g_0^{(0)},g_1^{(0)}\rangle = \begin{pmatrix} h_0^{(0)} \\ h_1^{(0)} \\ h_2^{(0)} \end{pmatrix}.$$

The exhaustive analysis of this problem would require a lot of space. Fortunately, it has already been performed elsewhere [8], with the most relevant result being that one just gets not more than two real solutions

$$|1,1\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad |-2,-2\rangle = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}. \tag{28}$$

They may be interpreted, as we already mentioned, as a doublet of the decadic quasi-exact large$-\ell$ bound states. In some applications, one also needs to find all the complex eigenvalues [21] . Although they would still be tractable by our present perturbation recipe, we shall ignore these solutions here as unphysical.

A.1. Left zero-order eigenvectors

The *left* eigenvectors of our perturbed as well as unperturbed Hamiltonians H may be found of interest as solutions compatible with the conjugate equation

$$\langle_\xi\langle g_0,g_1,\ldots,g_{q-1}|\, H = \langle_\xi\langle g_0,g_1,\ldots,g_{q-1}|\, S(g_0,g_1,\ldots,g_{q-1})\,. \tag{29}$$

In a double-bra Dirac-like notation, these row vectors $\langle_\xi\langle g_0,g_1,\ldots,g_{q-1}|$ are numbered by an additional subscript $\xi = 1,2,\ldots,\xi_{max}$. Such a convention emphasizes the ambiguity of the solutions.

Our special illustration $H^{(0)}$ of eq. (18) offers the respective symmetric and antisymmetric left eigenvector

$$\langle_1\langle 1,1| \equiv (1,1,1,1), \qquad \langle_2\langle 1,1| \equiv (3,-1,1,-3) \tag{30}$$

at $g_0 = g_1 = 1$, or

$$\langle_1\langle -2,-2| \equiv (2,-1,-1,2), \qquad \langle_2\langle -2,-2| \equiv (0,1,-1,0) \tag{31}$$

at $g_0 = g_1 = -2$. Arbitrary superpositions of these doublets may be employed instead. This reflects the incomplete (or rather *"under-complete"*) character of eq. (29).

A.2. Reduced zero-order eigenvectors

At any $q > 1$, one might prefer the choice of the row eigenvectors with as many zeros as possible. It is obvious that the linearly independent $q-$plets of the vectors of this type may be written as products

$$\langle_\xi\langle g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}| = \langle_j\langle \varrho(g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)})| \times \Pi_j, \qquad j = 1,2,\ldots,q \tag{32}$$

with $(N+1)\times(N+q)-$dimensional "reduction" matrices Π_j (= transpositions of some of the "unit-like" matrices $\mathcal{J}_{\xi'}$ with $\xi \neq j \neq \xi'$ in general).

In our example at $q = N = 2$, the sample of vectors in eq. (30) may be replaced by the mutually conjugate "reducible" eigenvectors $\langle_3\langle 1,1| \equiv (3,1,2,0)$ and $\langle_4\langle 1,1| \equiv (0,2,1,3)$. Their explicit reductions

$$\langle_3\langle 1,1| = (3,1,2)\times\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \langle_4\langle 1,1| = (2,1,3)\times\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

may be abbreviated as $\langle_3\langle 1,1| = \langle_1\langle \varrho(1,1)|\,\Pi_1$ and $\langle_4\langle 1,1| = \langle_2\langle \varrho(1,1)|\,\Pi_2$, respectively, with $\Pi_j = \mathcal{J}_j^T$.

A.3. Linearly independent sets

The reduced, $(N+1)-$dimensional "$\varrho-$vectors" $\langle_j\langle \varrho|$ may be interpreted as the left eigenvectors of the $(N+1)\times(N+1)-$dimensional *square* matrices $[\Pi_j\,(H_0 - S)]$. These reduced eigenvectors must exist and be nontrivial since all their "secular"

determinants vanish. In such a context, one may sometimes need to guarantee the linear independence of the row vectors at the first q subscripts $j = \xi = 1, 2, \ldots, q$ (say, by an appropriate re-numbering of their "overcomplete" available family).

Sometimes, we may have to make the choice of $\Pi_j = \mathcal{J}_{j'}^T$ with $j \neq j'$ for this purpose. For example, the mutually conjugate superpositions $\langle_3\langle -2, -2| \equiv (1, 0, -1, 1)$ and $\langle_4\langle -2, -2| \equiv (1, -1, 0, 1)$ of the states (31) lead to the respective factorizations

$$\langle_3\langle -2, -2| = (1, -1, 1) \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \langle_4\langle -2, -2| = (1, -1, 1) \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with the same form of the reduced array $\langle_1\langle \varrho(-2, -2)|$. Such a degeneracy reflects merely the presence of the random zeros in the antisymmetric vector in (31). It may be avoided easily since the relation $\langle_2\langle -2, -2| = (0, 1, -1)\,\Pi_1 \equiv (1, -1, 0)|\,\Pi_2$ gives the other two alternative options for the second and safely linearly independent reduced vector $\langle_2\langle \varrho(-2, -2)|$.

Appendix B. A few technical aspects of our innovated perturbation recipe

B.1. The explicit evaluation of the corrections to the perturbed energies and couplings

As long as our unperturbed Hamiltonian $H^{(0)}$ occurs also in eq. (23) which may be re-written in the form

$$\langle_j\langle \varrho(g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)})|\,\Pi_j\,\left(H^{(0)} - S^{(0)}\right) = 0\,, \qquad j = 1, 2, \ldots, q\,, \tag{33}$$

we may multiply eq. (26) by the set of matrices Π_j and by the independent vectors $\langle_j\langle \varrho\left(g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}\right)| \equiv \langle_j\langle \varrho|$ from the left. This leads to the system of relations

$$\langle_j\langle \varrho|\,\Pi_j\,S^{(k)}\,|\,0\rangle = -\langle_j\langle \varrho|\,\Pi_j\,|\,\text{known}^{(k-1)}\rangle\,, \qquad j = 1, 2, \ldots, q\,, \tag{34}$$

i.e., to an elementary $q-$dimensional matrix-inversion definition of the $k-$th-order energies/couplings $g_{\xi-1}^{(k)}$,

$$\sum_{\xi=1}^{q} \mathcal{F}_{j,\xi}^{(\text{known})}\,g_{\xi-1}^{(k)} = c_j^{(\text{known})}\,, \qquad j = 1, 2, \ldots, q\,. \tag{35}$$

Here, we merely introduced abbreviations $c_j^{(\rm known)} = -\langle_j\langle\varrho|\,\Pi_j\,|\,{\rm known}^{(k-1)}\rangle$ and $\mathcal{F}_{j,\xi}^{(\rm known)} = \langle_j\langle\varrho|\,[\Pi_j\,\mathcal{J}_\xi]\,|\,0\rangle$ for scalar products of two known vectors in $N+1$ dimensions. Their calculation may be facilitated by the evaluation of all the elements

$$[G_{j,\xi}]_{mn} = \sum_{k=1}^{N+q} [\Pi_j]_{mk}\,[\mathcal{J}_\xi]_{kn} \qquad\qquad m,n = 0,1,\ldots,N$$

in a preparatory step. One should remember that all the elements of both the non-square and sparse matrix factors are here equal to 0 or 1. The matrix elements of the product $\Pi_j\,\mathcal{J}_\xi$ will often vanish, therefore. In the generic case with $\Pi_j = \mathcal{J}_j^T$ we even get

$$(\,|j-\xi| \geq N+1\,) \quad\Longrightarrow\quad \mathcal{J}_j^T\,\mathcal{J}_\xi = 0\,. \tag{36}$$

This means that the sparse matrix $\mathcal{F}$ of the coupling-defining system (35) has a band-matrix structure and its inversion is easier.

B.2. Perturbed eigenvectors

Whenever the solution of the zero-order eq. (22) is unique, the ambiguity of the vector $|\,k\rangle$ specified by the $k-$th eq. (26) lies in an uncontrolled admixture of the $(N+1)-$dimensional zero-order vector $|\,0\rangle$. Once we construct any (normalized) basis in the corresponding $(N+1)-$dimensional space,

$$\{|\,\beta_m\rangle\}_{m=0}^{N}$$

and assume that the above vector coincides, say, with its zeroth element, $|\,0\rangle \equiv |\,\beta_0\rangle$, we may simply follow the textbooks and define the "right" projector

$$Q_R = \sum_{m=1}^{N} |\,\beta_m\rangle\,\langle\beta_m\,|$$

which mediates the standard Rayleigh-Schrödinger normalization of $|\,k\rangle = Q_R|\,k\rangle$.

In parallel, we have to recollect that we already employed q independent rows of the $k-$th eq. (26) for the specification of $S^{(k)}$ via eq. (35). More specifically, we multiplied eq. (26) by q vectors $\langle_j\langle\varrho|\,\Pi_j$ from the left. As long as these vectors were chosen as linearly independent, they span a $q-$dimensional subspace in the "larger", $(N+q)-$dimensional vector space. This allows us to assume that the orthogonal

complement of this subspace is spanned by an $N-$plet of some $(N+q)-$dimensional vectors $\mid \alpha_n\rangle$. These vectors define our second, "left" projector

$$Q_L = \sum_{n=1}^{N} \mid \alpha_n\rangle \, \langle \alpha_n \mid .$$

We are now ready to replace our non-homogeneous algebraic eq. (26) by its subsystem

$$Q_L \left[H^{(0)} - S^{(0)}\right] Q_R \mid k\rangle = Q_L |\, \text{known}^{(k-1)}\rangle + Q_L \, S^{(k)} \mid 0\rangle \tag{37}$$

where the second term on the right-hand side has been made "known" in the previous subsection. By construction, the left-hand-side N by N matrix is invertible and we have

$$\mid k\rangle = Q_R \, \frac{1}{Q_L \, [H^{(0)} - S^{(0)}] \, Q_R} \, Q_L \, \left(|\, \text{known}^{(k-1)}\rangle + S^{(k)} \mid 0\rangle\right) \tag{38}$$

which is our final and compact "generalized Rayleigh-Schrödinger" explicit formula for the $k-$th correction to the wave function.

B.3. Left perturbed eigenvectors

We have seen that in the Magyari-equation context, the left vectors only played a role in their *unperturbed*, zero-order form so that the description of their perturbation construction might simply be skipped as redundant. Nevertheless, for the sake of completeness, let us add a few remarks also on the $q-$plet of the row (left) eigenvectors of the non-square Hamiltonians and on all the space spanned by their superpositions

$$\langle\langle\psi| = \sum_{\xi=1}^{q} C_\xi \, \cdot \, \langle_\xi\langle g_0, g_1, \ldots, g_{q-1}| \, . \tag{39}$$

By assumption, they all satisfy the perturbed conjugate eq. (29) and we may expand both their separate components and the coefficients in the power series in λ. The combination of these series

$$\langle_\xi\langle g_0, g_1, \ldots, g_{q-1}| = \langle_\xi\langle g_0^{(0)}, g_1^{(0)}, \ldots, g_{q-1}^{(0)}| + \lambda \, \langle_\xi\langle g_0^{(1)}, g_1^{(1)}, \ldots, g_{q-1}^{(1)}| + \ldots \tag{40}$$

and $C_\xi = \sum_k \lambda^k \, C_\xi^{(k)}$ gives

$$\langle\langle\psi| = \sum_k \lambda^k \, \langle\langle\psi^{(k)}|, \qquad\qquad \langle\langle\psi^{(k)}| = \sum_{\xi=1}^{q} \sum_{n=0}^{k} C_\xi^{(k-n)} \cdot \langle_\xi\langle n \, | \tag{41}$$

where, in a naturally simplified notation, $\langle_\xi\langle n\,| \;\equiv\; \langle_\xi\langle g_0^{(n)}, g_1^{(n)}, \ldots, g_{q-1}^{(n)}|$.

Let us now enter the most characteristic postulate of *all* the Rayleigh-Schrödinger-type perturbation recipes which removes the ambiguity of the eigenvectors by the consequent requirement of a *complete absence* of any zero-order component $\langle_\xi\langle 0\,|$ in any correction $\langle\langle\psi^{(k)}|$ with $k \geq 1$.

In our present case this option leads to the two independent consequences. Firstly, in the light of eq. (41) we have to put $C_\xi^{(1)} = C_\xi^{(2)} = \ldots = 0$ [i.e., $n = k$ in eq. (41)] and get just $C_\xi \equiv C_\xi^{(0)}$. Secondly, *all* the vectors $\langle_\xi\langle n\,|$ must be constructed as perpendicular to *all* $\langle_j\langle 0\,|$ at *any* $n \geq 1$, i.e., in our notation of section 6.2,

$$\langle_\xi\langle n\,| = \langle_\xi\langle n\,|\,Q_L\,, \quad n = 1, 2, \ldots\,, \qquad \xi = 1, 2, \ldots, q\,. \tag{42}$$

With this normalization we may now insert eq. (41) in eq. (23) and arrive at an analogue of eq. (26). Of course, we may skip the repetition of the reconstruction of $S^{(k)}$ and jump immediately to the following $k \geq 1$ analogue of eq. (37),

$$\langle_\xi\langle k\,|\,Q_L\,\left[H^{(0)} - S^{(0)}\right] Q_R = \langle_\xi\langle\,\text{known}^{(k-1)}\,|\,Q_R, \qquad \xi = 1, 2, \ldots, q\,. \tag{43}$$

With

$$\langle_\xi\langle\,\text{known}^{(0)}\,| = \langle_\xi\langle 0\,|\,\left[S^{(1)} - H^{(1)}\right] \tag{44}$$

at $k = 1$ etc, the trivial N by N inversion gives the final formula

$$\langle_\xi\langle k\,| = \langle_\xi\langle\,\text{known}\,|\cdot Q_R\,\frac{1}{Q_L\,[H^{(0)} - S^{(0)}]\,Q_R}\,Q_L\,, \qquad \xi = 1, 2, \ldots, q\,. \tag{45}$$

The detailed account of our Magyari-inspired recurrent recipe is completed.